ADMINISTRATIVE INFORMATION

1. **Project Name:** Prediction of Corrosion of Advanced Materials and Fabricated Components

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5. **Date Project Initiated:** 11/17/2003

6. **Expected Completion Date:** 10/31/2006

PROJECT RATIONALE AND STRATEGY

7. **Project Objective:**

The goal of this project is to provide materials engineers, chemical engineers and plant operators with a software tool that will enable them to predict localized corrosion of process equipment including fabricated components as well as base alloys. For design and revamp purposes, the software will predict the occurrence of localized corrosion and guide the user to select the optimum alloy for a given environment. For the operation of existing plants, the software will enable the users to predict the remaining life of equipment and help in scheduling maintenance activities.

8. **Technical Barrier(s) Being Addressed:**

Over the last two decades, many advanced metallic materials have been developed for withstanding severe corrosion and erosion that are encountered in industrial processes. However, the application of these materials by industry has fallen far short of initial expectations because (i) their performance has been limited by fabrication processes, which are not considered in materials development and (ii) there has been a lack of tools to evaluate their performance in a given application prior to placing them in service. At present, there is no technically sound basis for judging the corrosion performance of these materials in real-world process environments without performing specific tests. Alloy designers and new process developers rely on standard laboratory tests, such as immersion tests in artificial seawater or ferric chloride to compare the performance of novel materials against previously used materials. These laboratory tests are not adequate for judging the true performance of fabricated materials in real-world environments. In some cases, pilot plant studies are conducted to select materials for the process. However, the pilot scale studies can be time-consuming and expensive.

9. **Project Pathway:**

This project combines fundamental understanding of mechanisms of corrosion with focused experimental results to predict the corrosion of advanced, base or fabricated, alloys in "real-world" environments encountered in the chemical industry. The program aims to develop a software tool that will make it possible to predict the corrosion performance of fabricated components in any environment utilizing a minimum data set. At the heart of this approach is the development of correlations between local compositions in the alloy with fundamental parameters that control the occurrence of localized corrosion. The fundamental parameters that dictate the occurrence of localized corrosion are the corrosion and repassivation potentials. The program team, OLI Systems and Southwest Research Institute, has developed theoretical models for these parameters. These theoretical models will be extended to predict the occurrence of localized corrosion of base materials, welds, weld overlays, and other fabrication operations in a variety of environments containing aggressive and non-aggressive species. The results of this project will reduce the barriers to the use of advanced materials in industry by allowing process designers and operators to evaluate these materials under realistic conditions of fabrication and in-service chemical environments. Users will also be able to identify process changes, corrosion inhibition strategies, and other control options before costly shutdowns, energy waste, and environmental releases occur. These innovative corrosion mitigation measures can be tested in a virtual laboratory without risking the plant. The "useful remaining life" will be able to be predicted based on operating experience and projected operating conditions so that catastrophic failures can be avoided and well-planned corrosion control and maintenance actions can be proactively scheduled.

10. **Critical Technical Metrics:**

Baseline metrics:

- A general method for predicting localized corrosion of base metals has been established and verified; however, the model has been parameterized only for a limited number of metal-environment combinations;
- A method has been established for extrapolating observed short-term corrosion damage into the future and predicting the remaining life.

Project metrics:

- Developing and verifying methodology for predicting the effect of complex chemistry, including multiple inhibiting ions, on the occurrence of localized corrosion;
- Constructing a model of localized corrosion of base alloys and fabricated materials that quantitatively agrees with results of standard tests;
- Constructing a methodology that quantitatively predicts the remaining life of fabricated components;
- Incorporating the methodology in CorrosionAnalyzer, a commercial software product.

PROJECT PLANS AND PROGRESS

11. **Past Accomplishments:**

This project partially continues a project titled "Performance Prediction Tool for Process Equipment Subject to Localized Corrosion", which was funded by ATP from 11/2000 to 10/2003. In that project, OLI Systems and Southwest Research Institute have developed methods to:

- Predict whether or not localized corrosion of base metals will occur in an aqueous environment. This has been implemented in software that can help design systems that do not suffer from localized corrosion.
- Predict the long-term damage due to localized corrosion on the basis of short-term inspection results. This is particularly useful for the operation and maintenance of existing systems and will predict the useful lifetime of equipment, as long as process conditions do not change during the lifetime of the equipment.

During the first six months of this project, the project team has accomplished the following:

- The experimental test matrix has been designed. In particular, the alloys, treatment methods and representative process environments have been selected and the experiments have been initiated.
- Model parameters have been developed for predicting the general corrosion and the occurrence of localized corrosion for alloys C-22 and C-276. The model predictions have been extensively verified against experimental data from SwRI measurements as well as literature sources. Excellent agreement with the data has been obtained.
- Methodology has been developed for determining parameters for predicting the evolution of corrosion damage using extreme value statistics combined with damage function analysis. This sets the stage for predicting the effects of changing process conditions on the evolution of corrosion damage.

12. **Future Plans:**

The major milestones that remain to be accomplished are:

1. Correlation of fabrication process parameters with microchemistry (10/04)
2. Completion of microchemistry database (12/05)
3. Correlation of microchemistry with electrochemical data for selected systems (12/04)
4. Completion of electrochemical database (7/06)
5. Correlation of electrochemistry, microchemistry, propagation and standard test data (5/05)
6. Completion of growth and distribution database (1/06)
7. Reproducing corrosion potential data for various alloys (12/04)
8. Full parameterization of the general corrosion model (9/06)
9. Reproducing the effects of alloy chemistry on the repassivation potential (4/05)
10. Full parameterization of the repassivation potential model
11. Extension of the probabilistic damage function methodology to fabricated materials (12/04)
12. Verification of probabilistic damage function predictions (3/06)
13. Development of a software prototype (4/06)
14. Preliminary release of the software to industrial team members (4/06)
15. Feedback from team members and refinement of the software (9/06)

13. **Project Changes:** None so far.

14. **Commercialization Potential, Plans, and Activities:**

The primary vehicle for the commercialization of this technology will be OLI Systems' CorrosionAnalyzer, a software tool that is currently used, in a more limited version, by many companies in the chemical process industry. The capabilities of the CorrosionAnalyzer will be dramatically enhanced as a result of this project. In process design, the results of this project (encapsulated in the CorrosionAnalyzer) will provide the industry with (1) reliable prediction of the tendency of base alloys for localized corrosion; (2) a quantification of the difference in corrosion resistance of the base metal and weld; (2) insight into the behavior of over-alloyed filler metal, and how to design for these situations, and 3) understanding of how to select materials. In process operations, the software will help to predict the remaining useful life of the equipment. As industrial and infrastructural systems age (pipelines, refineries, power plants, etc.), this will address the considerable economic incentive to avoid unscheduled outages and to extend operation beyond the design lifetime.

Commercialization of the technology will involve the following:

1. *Software development with functions and GUI features defined by the prospective users.* OLI has substantial experience here and has already developed a commercial corrosion software product. The industrial team members will ensure that the resulting software meets the needs of the chemical process industry.
2. *Establishing an effective channel to the market.* OLI will utilize its existing network of worldwide agents, strong, established client relationships, and marketing partners. One of OLI's principal strengths is its extensive penetration of the major companies comprising the CPI, currently exceeding 75 major CPI companies. At least 50% of OLI's current client base are prospects for the products developed in this project. The existing client relationships are an immediate pathway to commercialization of the proposed products.
3. *Technology transfer through the industry groups, technical papers, professional association meetings.* OLI has a working relationship with MTI (Materials Technology Institute) and regularly publishes in peer-reviewed journals and through NACE meetings. OLI provides periodic free regional seminars to inform and educate the industry.
4. *Establishment of software training courses and dedicated customer technical support.* This is a normal business routine for OLI. OLI has an excellent reputation in these areas.
5. *Technical service.* Based on the software, technical services will be offered to the industry on a project basis.

15. **Patents, Publications, Presentations:** *The presentation below is based on the results of a previous project that are directly relevant to this project; Papers based on the current project are in preparation.*

A. Anderko, N. Sridhar, C.S. Brossia and D.S. Dunn, "A Computational Approach to Predicting the Occurrence of Localized Corrosion in Multicomponent Aqueous Solutions", paper no. 04061, CORROSION/2004, New Orleans, LA, March 28 – April 1, 2004.